Principal Component Analysis of Mineral Abundances at IODP Site U1387

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Abstract

The Integrated Ocean Drilling Program embarked on Expedition 339 to examine sediment records from the Gulf of Cadiz for the history of Mediterranean Water Outflow and its effects. Studies by previous Ohio State University students have focused on the glacial and interglacial cycles of samples retrieved from Site U1387, which were drilled during Expedition 339. Studies of the cycles used semi-quantitative mineral abundance data (peak areas on x-ray diffractograms) and identified different patterns of mineral variability during two different time periods studied. The objective of this study was to evaluate these two sets of data in more detail, to see if a statistical analysis supported the conclusions of the original studies. Principal Component Analysis was run on each set of mineral peak area data separately so that the principal components defined, as well as the loadings of each mineral on the principal components, could be compared. The principal components defined, as well as their mineral loadings, proved that the separate sets of data exhibited different patterns of variability. Although all principal components are consistent with biogenic input of carbonate and detrital input from the Iberian Peninsula, the difference in results may reflect environmental and oceanographic changes in this region across the Mid-Pleistocene Transition, an event that lengthened glacial/interglacial cycles from 41,000 year periodicity to 100,000 year periods.

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Introduction

The International Ocean Drilling Program (IODP) was a program focused on examining and exploring the oceans to learn more about Earth's geologic history and processes. IODP Expedition 339 was conducted to recover and examine sedimentary records of Mediterranean Outflow Water (MOW) and its effect on global circulation and climate (Expedition 339 Scientists, 2013). During Expedition 339, scientists drilled at multiple locations in the Gulf of Cadiz as shown in Figure 1. Site U1387 was one of five sites drilled in the Gulf of Cadiz, and provided the samples used in this study.

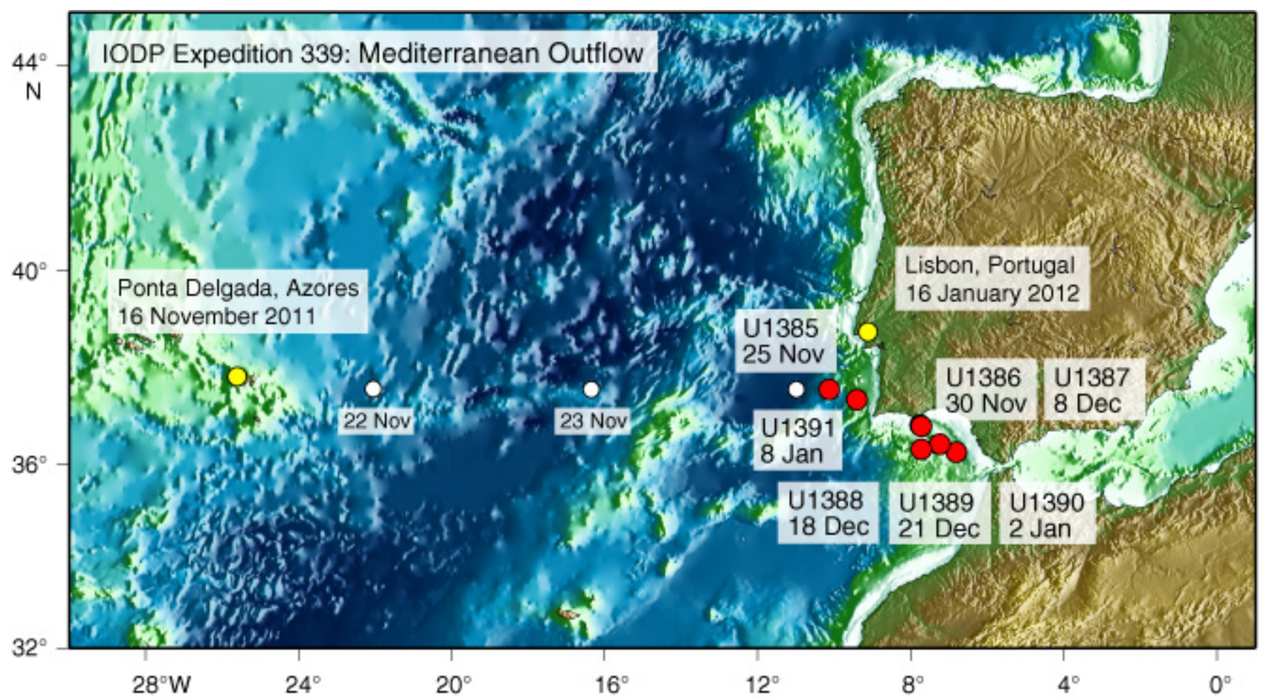

Figure 1: IODP Expedition 339 Site Map. From Expedition 339 Scientists(2013)

Huston (2015) and O'Brien (2014) previously examined samples from Site U1387. Huston (2015) examined the mineralogy of samples aged 1.014 to 1.236 mya at Site U1387. The goal of her work was to examine variations in mineral content through a glacial/interglacial cycle (Huston, 2015). O'Brien (2014) examined the mineralogy of samples aged 178.76 to 304.57 kya, also at Site U1387. The objective of his study, as stated in his study goals, “was to employ mineralogy to interpret shifts in MOW position in the Gulf of Cadiz from recent to ~300 kya” (O’Brien, 2014).

The goal of this study is to examine the data generated by Huston (2015) and O’Brien (2014) at Site U1387 to determine the similarities and/or differences in patterns of mineral abundance variation over the intervals that Huston (2015) and O’Brien (2014) examined. Both studies utilized mineral peak area data, meaning the variations in mineral abundance can be examined relative to each other. With principal component analysis, this thesis will test the hypothesis that the patterns of mineral supply and variability were similar over the two time intervals examined by Huston (2015) and O’Brien (2014) at Site U1387.

Methods

The two sets of samples analyzed in this study were collected from Site U1387 in the Gulf of Cadiz. The ages of samples in Set 1 ranged from 178.76 to 304.57 kya (thousands of years ago) while the ages of the second set ranged from 1.014 to 1.236 mya (millions of years ago). The mineral peak intensity data used in this study were generated by X-ray diffraction (XRD) techniques on a set of 13 samples (Set 1; O'Brien, 2014) and a second set of 25 samples (Set 2; Huston, 2015). Both sets of samples were analyzed using the PANalytical X'Pert Pro XRD in the Subsurface Energy Materials Characterization & Analysis Laboratory (SEMCAL) in the School of Earth Sciences at Ohio State University. The analytical methods are described in O'Brien (2014) and Huston (2015), and the resulting data are presented in Appendix B of O'Brien (2014), and Table 2 of Huston (2015).

For this study, these two data sets were analyzed separately using the PAST software, which can be downloaded for no cost at http://folk.uio.no/ohammer/past/. The mineral peak intensity data were imported into the software, with the sample depths and ages omitted to allow for an accurate analysis. The format of data entry into PAST is similar to an Excel worksheet, allowing for rows and columns of data to be analyzed in univariate or multivariate methods. Once both sets of data were imported and formatted in PAST, a Principal Component Analysis (PCA) was conducted. By highlighting the data to be used, the PCA can be done on each sample set individually. Under the Multivariate tab and Ordination subgroup, "Principal Component (PCA)" was selected. This produced the eigenvalues, scatterplots, loadings, loading plots, and screen plots resulting from the analysis of that set of data.

Results

Principal component analysis was run separately on the two sets of data from different age/depth intervals of Site U1387. For each set of data, the PCA defined five principal components, which accounted for 100% of the total variance in the data set. Each principal component is defined by a loading on each mineral, and the loadings for that principal component define a co-varying assemblage of minerals (quartz, calcite, dolomite, illite, and a mix of chlorite/kaolinite/smectite (7Å)). For both data sets, principal components 1 and 2 accounted for >90% of the respective total variance, reaching 98.3% of the variance for Sample Set 1 and 90.5% of the variance for Sample Set 2. Since 90% of the variance for each sample set is explained by the first two principal components, only Components 1 and 2 will be discussed when examining each data set. Table 1 presents the variance explained by each principal component from the analysis of Sample Set 1. Table 2 presents the loadings of each mineral on each principal component defined for Sample Set 1. Table 3 presents the variance explained by each principal component from the analysis of Sample Set 2. Table 4 presents the loadings of each mineral on each principal component defined for Sample Set 2.

For Sample Set 1, Principal Component 1 (PC 1) explained 87.4% of the original total data variance. Principal Component 1 is defined by a high positive loading on calcite (Fig. 2). Loadings on the other minerals were low and negative, meaning that calcite was the dominant mineral in PC 1 of Set 1. Principal Component 2 (PC 2) explained 10.8% of Set 1's total variance. The second component is defined by a high positive loading on dolomite, with lower positive loadings on quartz and illite (Fig. 3).

In the analysis of Sample Set 2, Principal Components 1 and 2 explain relatively similar amounts of the total data variance. Principal Component 1 accounted for 46.5% of the total variance in Set 2 and is defined by a high positive loading on dolomite, and a high negative loading on calcite (Fig. 4). Principal Component 2 explained 43.9 % of the total data variance in Sample Set 2, with similar high positive loadings on both calcite and dolomite (Fig. 5).

PC	Eigenvalue	% variance
1	64666.8	87.442
2	8009.81	10.831
3	649.754	0.8786
4	370.332	0.50076
5	256.992	0.3475

Table 1: Principal Component Analysis of Sample Set 1

	PC 1	PC 2	PC 3	PC 4	PC 5
Quartz	-0.04114	0.23984	-0.62287	0.57396	0.47263
Calcite	0.99154	0.122	0.011394	-0.00267	0.042651
Dolomite	-0.10987	0.9376	-0.01381	-0.29709	-0.14276
Illite	-0.03664	0.22022	0.73007	0.64238	0.067095
7Å	-0.04166	0.000599	0.28055	-0.41187	0.86598

Table 2: Loadings of Sample Set 1

PC	Eigenvalue	% variance
1	43085.6	46.561
2	40702.5	43.986
3	4111.09	4.4427
4	3520.11	3.804
5	1116.74	1.2068

Table 3: Principal Component Analysis of Sample Set 2

	PC 1	PC 2	PC 3	PC 4	PC 5
Quartz	0.19512	0.13737	-0.29331	0.92541	-0.02546
Calcite	-0.69787	0.70565	0.089049	0.071836	0.044042
Dolomite	0.6823	0.69185	0.047505	-0.2313	0.007486
Illite	0.08454	-0.06379	0.63191	0.21223	0.73785
7Å	0.047226	-0.02126	0.71026	0.19981	-0.673

Table 4: Loadings of Sample Set 2

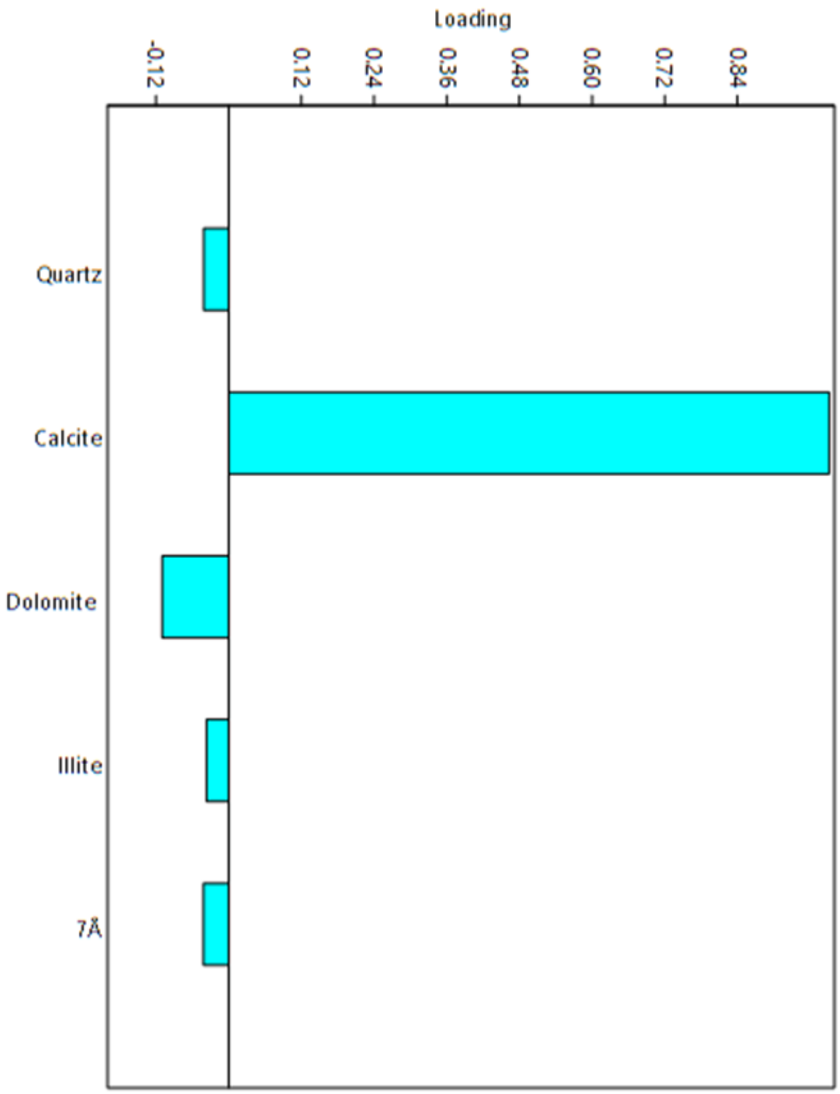

Figure 2: Loadings Plot of Principal Component 1 of Set 1

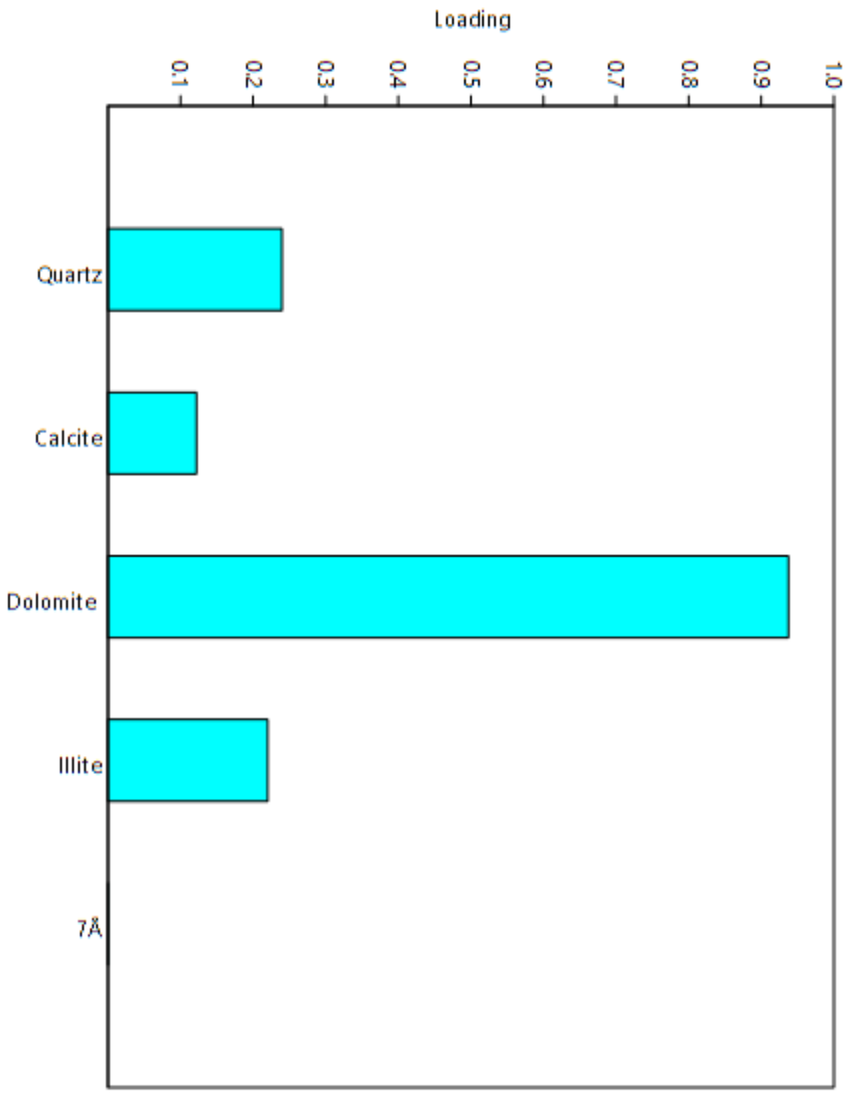

Figure 3: Loadings Plot of Principal Component 2 of Set 1

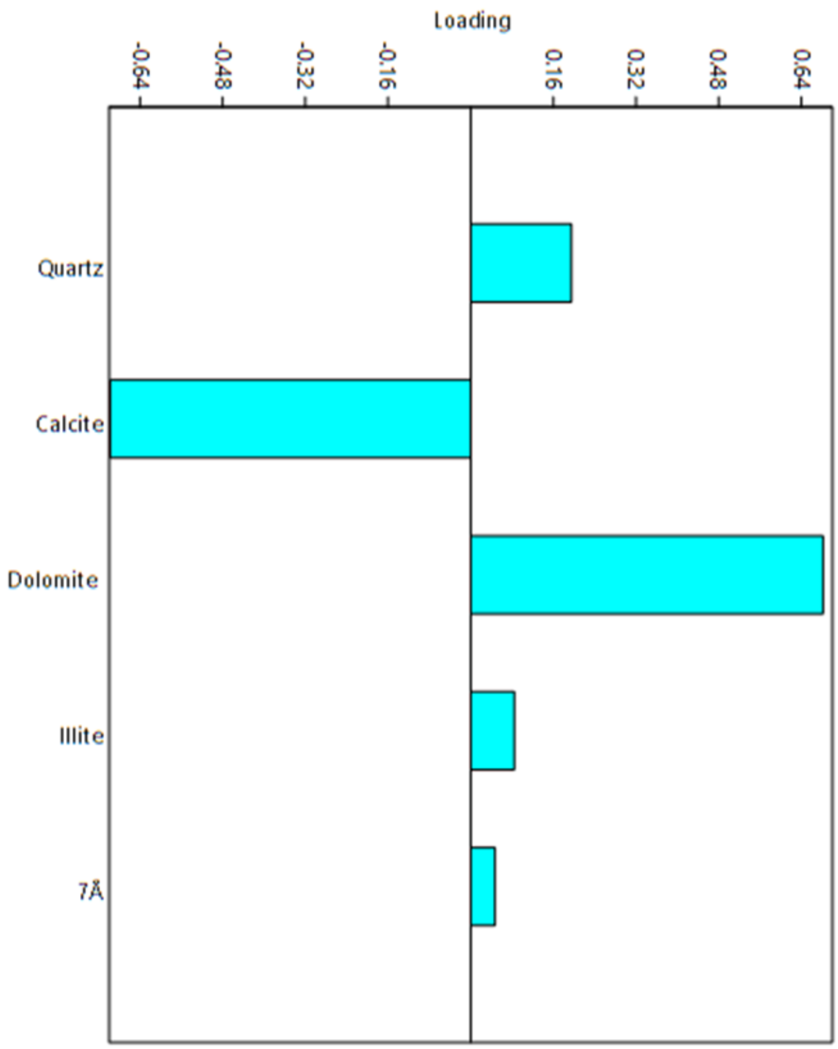

Figure 4: Loadings Plot of Principal Component 1 of Set 2

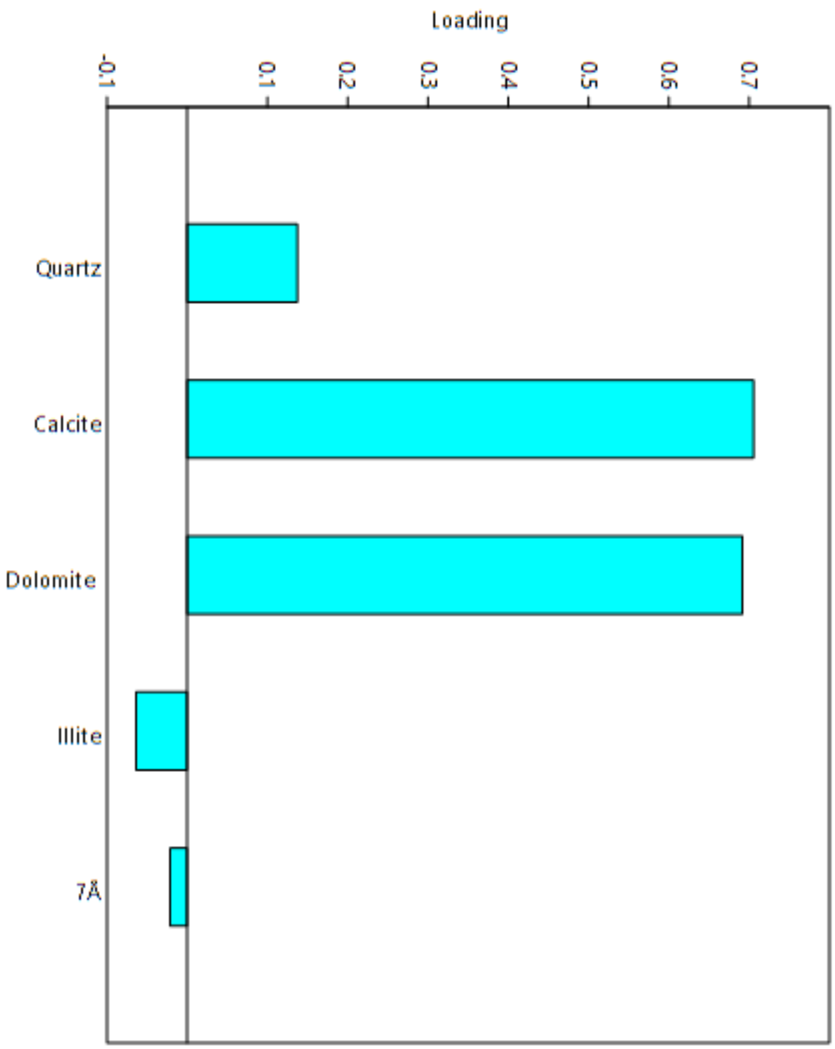

Figure 5: Loadings Plot of Principal Component 2 of Set 2

Discussion

The two sets of data came from different depths in Site U1387. Principal Component Analysis of each data set separately has defined distinctly different principal components, both in terms of the variance explained and the loadings on each principal component. Analysis of Sample Set 1 yielded a high calcite loading on the first component and high dolomite loadings on the second component. Since the calcite loading on PC 1 is not matched by any other loading of equivalent magnitude, PC 1 is interpreted to indicate the presence or absence of carbonate. Carbonate in marine sediments can be detrital, or it can be supplied by contemporaneous marine life (i.e., be biogenic). Detrital carbonate would be expected to be accompanied by an input of other detrital minerals, but that association is not indicated by loadings on PC 1. As result, the carbonate influence indicated by PC 1 is interpreted to reflect the presence or absence of biogenic material (e.g., marine microfossils). In contrast, PC 2 is defined by a large positive loading on dolomite, with other lower positive loadings of minerals that obviously are detrital. As a result, the association of dolomite, quartz and illite of a detrital origin defined by PC 2 is interpreted to reflect detrital supply. This mineral assemblage is consistent with the geology of the southwest Iberian Peninsula.

The analysis of data from Sample Set 2 defined two principal components that explain similar amounts of variance. PC 1 is defined by a high negative loading on calcite and a high positive loading on dolomite. This inverse relationship of loadings indicates an inverse relationship between calcite and dolomite abundances, suggesting detrital supply of dolomite and biogenic supply of some calcite. PC 2 had high positive loadings for both calcite and dolomite which suggests that some calcite in Sample Set 2 was also detrital.

The results of the principal component analyses are quite different for Sample Set 1 and Sample Set 2, in terms of both the distribution of variance explained by each principal component and the mineral loadings on each component. For Set 1, PC 1 explains almost 90% of the total data variance and is dominated solely by calcite of inferred biogenic origin. For Set 2, PC 1 explains ~46% of the total variance, and records an inverse relationship between detrital dolomite and biogenic calcite. PC 2 of Set 1 records detrital supply, but accounts for only ~10% of the data variance. In contrast, PC 2 of Set 2 also appears to record detrital supply but explains ~44% of the data variance.

In summary, the analysis of Sample Set 2 appears to indicate that the older record from Site U1387 was more affected by variations in detrital supply than the younger record was. Although the exact reasons for this change cannot be defined by this study, the changes identified here may be part of the local or regional expression of the Mid-Pleistocene Transition, when glacial/interglacial cycles changed from the older 41ky periodicity to the younger 100ky cycles (Clark et al., 2006).

Conclusions

This study analyzed mineral peak area data (i.e., semi-quantitative mineral abundances) provided by previous examinations of material from the two age intervals of Site U1387. The objective of this study was to determine whether the patterns of mineral deposition were different for these two intervals. Each data set was examined by Principal Component Analysis, with markedly different results for each data set. Although two principal components explained 90% or greater of the data variance for each data set, the distribution of variance explained was quite different for each data set. The definition of these two principal components, as indicated by mineral loadings on each, was also quite different for these two data sets. These results may reflect local or regional effects of the Mid-Pleistocene Transition, which occurred between the deposition of Sample Set 1 and the deposition of Sample Set 2. The Mid-Pleistocene Transition, which altered the pattern of glacial/ interglacial cycles, may have produced local/regional environmental and/or oceanographic changes that affected the patterns of mineral supply to Site U1387.

Recommendations for Future Work

One possible recommendation for future work would be continued study of Site U1387. Samples could be examined from ages closer to the start and end of the Mid-Pleistocene Transition. Data older than the Mid-Pleistocene Transition could be compared to those of Huston (2015) to determine if the mineral abundance variations are similar, while data younger than the Mid-Pleistocene Transition could be compared to those of O'Brien (2014). The data could help strengthen the explanation that the Mid-Pleistocene Transition was the time of the changes identified in this study.

Another possible recommendation for future work would involve the examination of mineral abundance data from other sites within the Gulf of Cadiz. Expedition 339 drilled five sites in the Gulf of Cadiz, meaning there are other sediment records available that could be examined for similar behavior (Expedition 339 Scientists, 2013). Examination of sediments with ages similar to those of Huston (2015) and O'Brien (2014) could help confirm the interpretation made by this study, or lead toward another interpretation.

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